A Unified Variational Approach to data analysis
Dynamic programming procedure

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A unified variational approach to data analysis.

Source data array

$$Y = (y_t, t \in T), y \in \mathcal{Y}$$

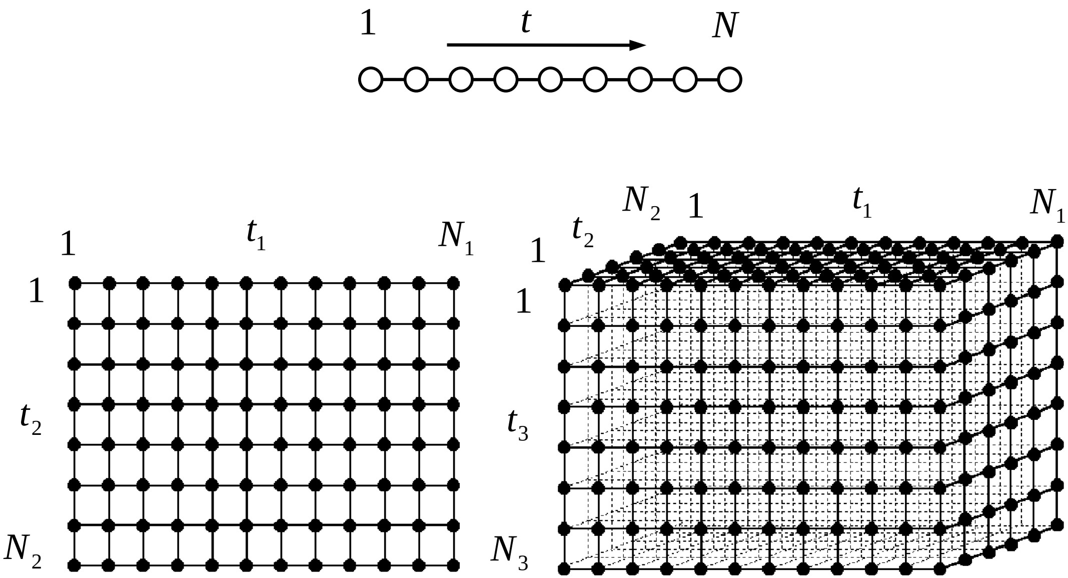
Result of processing

$$X = (x_t, t \in T), \; x \in \mathcal{X}$$

The original problem of data analysis can be turned to that of minimization of an appropriate objective function $J(X \mid Y)$ defined on the whole variety of possible results:

$$\hat{X}(Y) = \arg\min_{x_t \in \mathcal{X}} J(X \mid Y)$$

Adjacency graphs on the set of data array elements



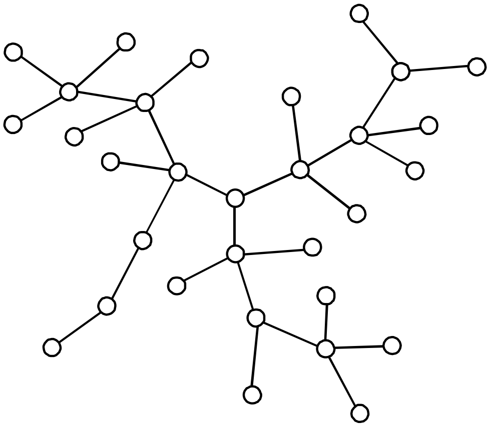
Pairwise separable objective function

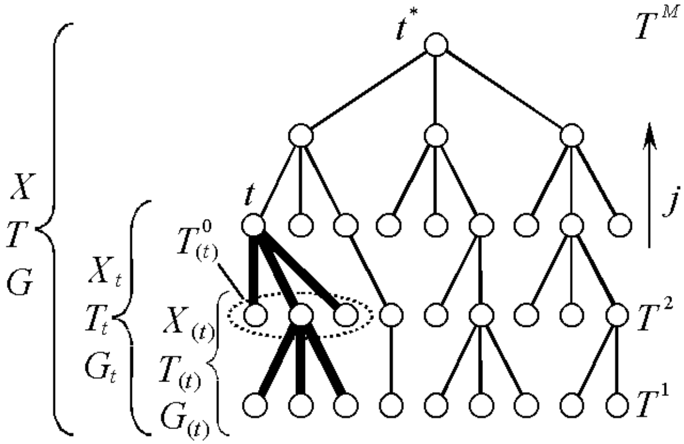
$$J(X\,|\,Y)=\sum_{t\in T}\psi_t(x_t\,|\,Y_t)+\sum_{(t',t'')\in G}\gamma_{t't''}(x_{t'},x_{t''})$$

$\psi_t(x_t\,|\,Y_t)$ – *node functions* which are meant to take the greater value the more evident is the contradiction between the hypothesis that x_t is just the “correct” local value we are seeking and the correspondent fragment Y_t of the source data array,

$\gamma_{t't''}(x_{t'},x_{t''})$ – *edge functions* that take the greater values the greater is the discrepancy between their arguments.

Hierarchical representation of a tree-like adjacency graph





Partial objective function defined on the descendant tree of node t

$$J_t(X_t) = \sum_{s \in T_t} \psi_s(x_s) + \sum_{(s',s'') \in G_t} \gamma_{s's''}(x_{s'}, x_{s''})$$

$$J_t(X_t) = J_t(x_t, X_{(t)}) = \psi_t(x_t) + \sum_{s \in T^0_{(t)}} \gamma_{ts}(x_t, x_s) + \sum_{s \in T^0_{(t)}} J_s(X_s) = \psi_t(x_t) + \sum_{s \in T^0_{(t)}} \left\{ \gamma_{ts}(x_t, x_s) + J_s(X_s) \right\}$$

Bellman functions

$$\tilde{J}_t(x_t) = \min_{X_{(t)}} J_t(x_t, X_{(t)}) = \psi_t(x_t) + \min_{x_s, X_{(s)}, s \in T^0_{(t)}} \sum_{s \in T^0_{(t)}} \left\{ \gamma_{ts}(x_t, x_s) + J_s(x_s, X_{(s)}) \right\}$$

Fundamental property of Bellman functions (upward recurrent relation)

$$\tilde{J}_t(x_t) = \psi_t(x_t) + \sum_{s \in T^0_{(t)}} \min_{x_s} \left\{ \gamma_{ts}(x_t, x_s) + \tilde{J}_s(x_s) \right\}$$

Downward recurrent relations

$$\tilde{x}_s(x_t) = \arg\min_{x_s} \left\{ \gamma_{ts}(x_t, x_s) + \tilde{J}_s(x_s) \right\}, \; s \in T^0_{(t)}$$

Marginal node functions

$$\hat{J}_t(x_t) = \min_{x_s,\, s \in T,\, s \neq t} J(X)$$

$$\hat{J}_s(x_s) = \min_{x_t} \left\{ \hat{J}_t(x_t) + \left[\tilde{J}_s(x_s) + \gamma_{ts}(x_t, x_s) \right] - \min_{x'_s} \left[\tilde{J}_s(x'_s) + \gamma_{ts}(x_t, x'_s) \right] \right\}, \; s \in T^0_{(t)}$$

Algorithm of objective function minimization

Ascending pass:

calculate and remember all the Bellman functions starting with Bellman functions for leaves $\tilde{J}_t(x_t) = \psi_t(x_t)$.

$$\tilde{J}_t(x_t) = \psi_t(x_t) + \sum_{s \in T^0_{(t)}} \min_{x_s} \left\{ \gamma_{ts}(x_t, x_s) + \tilde{J}_s(x_s) \right\}$$

Descending pass:

calculate optimal variable values or marginal functions for all the nodes starting with the root, where the marginal function coincides with the Bellman function $\hat{J}_{t^*}(x_{t^*}) = \tilde{J}_{t^*}(x_{t^*})$ and its minimization gives the optimal value at the root

$\hat{x}_{t^*} = \arg\min_{x_{t^*}} \tilde{J}_{t^*}(x_{t^*})$

$$\hat{J}_s(x_s) = \min_{x_t} \left\{ \hat{J}_t(x_t) + \left[\tilde{J}_s(x_s) + \gamma_{ts}(x_t, x_s) \right] - \min_{x'_s} \left[\tilde{J}_s(x'_s) + \gamma_{ts}(x_t, x'_s) \right] \right\},\ s \in T^0_{(t)}$$

Parametric family of quadratic functions for the case of continuous variables

Source data array	$Y=(y_t,\, t\in T),\, y\in \mathscr{Y}$
Result of processing	$X=(\mathbf{x}_t,\, t\in T),\ \mathbf{x}_t\in \mathrm{R}^n$
Quadratic node functions	$\psi_t(\mathbf{x}_t)=b_t^0+(\mathbf{x}_t-\mathbf{x}_t^0)^T\mathbf{Q}_t^0(\mathbf{x}_t-\mathbf{x}_t^0)$
Quadratic edge functions	$\gamma_{t't''}(\mathbf{x}_{t'},\mathbf{x}_{t''})=(\mathbf{x}_{t'}-\mathbf{x}_{t''})^T\mathbf{U}_{t't''}(\mathbf{x}_{t'}-\mathbf{x}_{t''})$
Pairwise separable quadratic objective function	$J(X)=\sum_{t\in T}\Big(b_t^0+(\mathbf{x}_t-\mathbf{x}_t^0)^T\mathbf{Q}_t^0(\mathbf{x}_t-\mathbf{x}_t^0)\Big)+\sum_{(t',t'')\in G}(\mathbf{x}_{t'}-\mathbf{x}_{t''})^T\mathbf{U}_{t't''}(\mathbf{x}_{t'}-\mathbf{x}_{t''})$

Parametric dynamic programming procedure for quadratic pairwise separable objective functions

Ascending pass: Bellman functions $\tilde{J}_t(\mathbf{x}_t)=\tilde{b}_t+(\mathbf{x}_t-\tilde{\mathbf{x}}_t)^T\tilde{\mathbf{Q}}_t(\mathbf{x}_t-\tilde{\mathbf{x}}_t)$ are calculated.

$$\tilde{\mathbf{Q}}_t=\mathbf{Q}_t^0+\sum_{s\in T_{(t)}^0}\tilde{\mathbf{Q}}_s\left(\tilde{\mathbf{Q}}_s+\mathbf{U}_{ts}\right)^{-1}\mathbf{U}_{ts},$$

$$\tilde{\mathbf{x}}_t=\tilde{\mathbf{Q}}_t^{-1}\left\{\mathbf{Q}_t^0\mathbf{x}_t^0+\sum_{s\in T_{(t)}^0}\tilde{\mathbf{Q}}_s\left(\tilde{\mathbf{Q}}_s+\mathbf{U}_{ts}\right)^{-1}\mathbf{U}_{ts}\tilde{\mathbf{x}}_s\right\},$$

$$\tilde{b}_t=b_t^0+(\mathbf{x}_t^0-\tilde{\mathbf{x}}_t)^T\mathbf{Q}_t^0\mathbf{x}_t^0+\sum_{s\in T_{(t)}^0}\left\{\tilde{b}_s+\left(\mathbf{x}_t-\tilde{\mathbf{x}}_s\right)^T\tilde{\mathbf{Q}}_s\left(\tilde{\mathbf{Q}}_s+\mathbf{U}_{ts}\right)^{-1}\mathbf{U}_{ts}\tilde{\mathbf{x}}_s\right\},$$

starting with the leaves, where $\tilde{J}_t(X_t)=\psi_t(x_t)$ and, consequently, $\tilde{\mathbf{x}}_t=\mathbf{x}_t^0$, $\tilde{b}_t=b_t^0$, $\tilde{\mathbf{Q}}_t=\mathbf{Q}_t^0$

Descending pass: marginal node functions $\hat{J}_t(\mathbf{x}_t)=\hat{b}+(\mathbf{x}_t-\hat{\mathbf{x}}_t)^T\hat{\mathbf{Q}}_t(\mathbf{x}_t-\hat{\mathbf{x}}_t)$ are calculated

$$\hat{b}=\tilde{b}_{t^*}$$

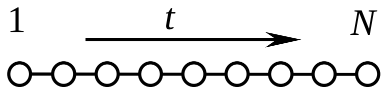
$$\hat{\mathbf{x}}_s=\tilde{\mathbf{x}}_s(\mathbf{x}_t)=(\mathbf{I}-\tilde{\mathbf{H}}_s)\tilde{\mathbf{x}}_s+\tilde{\mathbf{H}}_s\mathbf{x}_t=\tilde{\mathbf{x}}_t+\tilde{\mathbf{H}}_s(\mathbf{x}_t-\tilde{\mathbf{x}}_s),$$

$$\hat{\mathbf{Q}}_s=[\tilde{\mathbf{H}}_s\hat{\mathbf{Q}}_t^{-1}\tilde{\mathbf{H}}_s^T+(\tilde{\mathbf{Q}}_s+\mathbf{U}_{ts})^{-1}]^{-\mathbf{1}},$$

$$\tilde{\mathbf{H}}_s=(\tilde{\mathbf{Q}}_s+\mathbf{U}_{ts})^{-\mathbf{1}}\mathbf{U}_{ts}=(\mathbf{U}_{ts}^{-1}\tilde{\mathbf{Q}}_s+\mathbf{I})^{-1},\ s\in T_{(t)}^0,$$

starting from the root, where $\hat{J}_{t^*}(\mathbf{x}_{t^*})=\tilde{J}_{t^*}(\mathbf{x}_{t^*})$ and, hence, $\hat{\mathbf{x}}_{t^*}=\tilde{\mathbf{x}}_{t^*}$, $\hat{\mathbf{Q}}_{t^*}=\tilde{\mathbf{Q}}_{t^*}$.

Parametric dynamic programming procedure "forward and back" for signal analysis



Node functions $\psi_t(\mathbf{x}_t) = b_t^0 + (\mathbf{x}_t - \mathbf{x}_t^0)^T \mathbf{Q}_t^0 (\mathbf{x}_t - \mathbf{x}_t^0)$

Edge functions $\gamma_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = (\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t)^T \mathbf{U}_t (\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t)$

Pairwise separable quadratic objective function $J(X) = \sum_{t=1}^{N} \Big(b_t^0 + (\mathbf{x}_t - \mathbf{x}_t^0)^T \mathbf{Q}_t^0 (\mathbf{x}_t - \mathbf{x}_t^0) \Big) + \sum_{t=2}^{N} \Big((\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t)^T \mathbf{U}_t (\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t) \Big)$

First (forward) pass along the signal $t = 1, \ldots, N$: parameters of Bellman functions are calculated

$$\tilde{\mathbf{Q}}_t = \mathbf{Q}_t^0 + \mathbf{A}^T \left(\tilde{\mathbf{Q}}_{t-1}^{-1} + \mathbf{U}_t^{-1} \right)^{-1} \mathbf{A},$$

$$\tilde{\mathbf{x}}_t = \tilde{\mathbf{Q}}_t^{-1} \left\{ \mathbf{Q}_t^0 \mathbf{x}_t^0 + \mathbf{A}^T \left(\tilde{\mathbf{Q}}_{t-1}^{-1} + \mathbf{U}_t^{-1} \right)^{-1} \tilde{\mathbf{x}}_{t-1} \right\},$$

$$\tilde{b}_t = b_t^0 + \tilde{b}_{t-1} + (\mathbf{x}_t^0 - \tilde{\mathbf{x}}_t)^T \mathbf{Q}_t^0 \mathbf{x}_t^0 + \left(\tilde{\mathbf{x}}_{t-1} - \mathbf{A}\mathbf{x}_t \right)^T \left(\tilde{\mathbf{Q}}_{t-1}^{-1} + \mathbf{U}_t^{-1} \right)^{-1} \tilde{\mathbf{x}}_{t-1},$$

the first sample is the only leaf $t = 1$: $\tilde{b}_1 = b_1^0$, $\tilde{\mathbf{x}}_1 = \mathbf{x}_1^0$, $\tilde{\mathbf{Q}}_1 = \mathbf{Q}_1^0$.

Second (backward) pass $t = N, \ldots, 1$: parameters of marginal node functions are computed

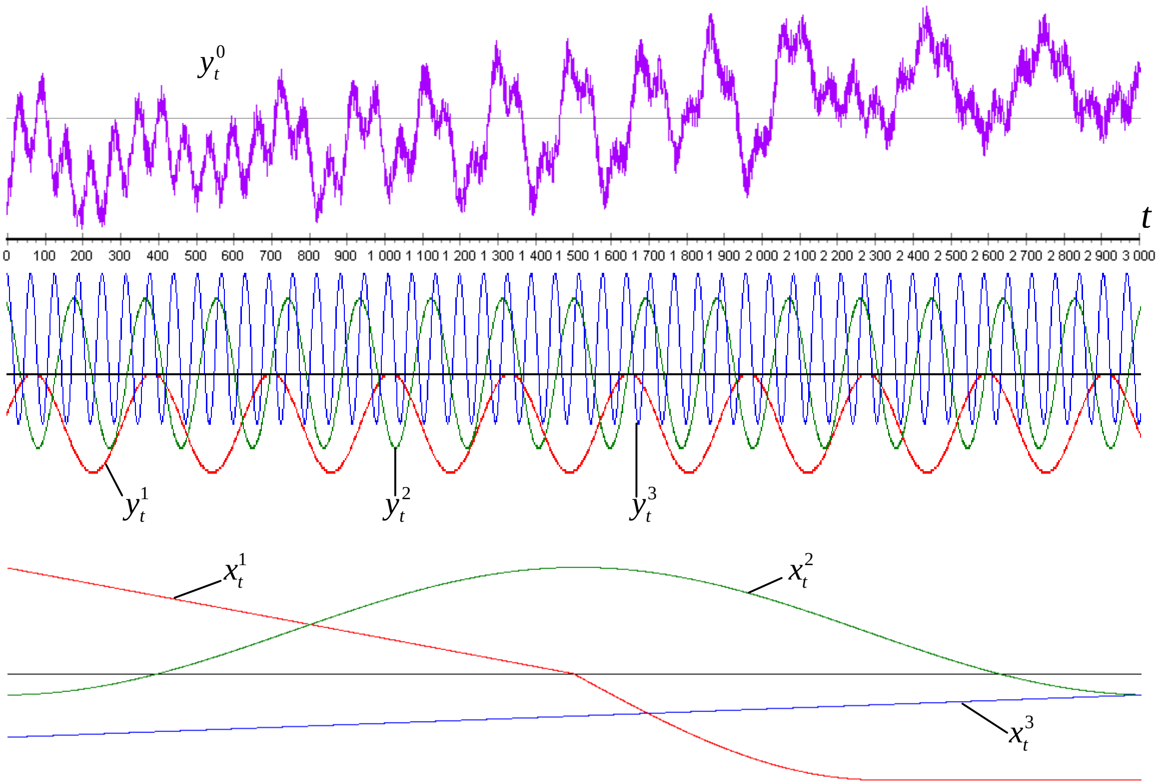
$$\hat{\mathbf{x}}_{t-1} = (\mathbf{I} - \tilde{\mathbf{H}}_{t-1}) \tilde{\mathbf{x}}_{t-1} + \tilde{\mathbf{H}}_{t-1} \mathbf{A}\mathbf{x}_t = \tilde{\mathbf{x}}_{t-1} + \tilde{\mathbf{H}}_{t-1} (\mathbf{A}\mathbf{x}_t - \tilde{\mathbf{x}}_{t-1})$$

$$\hat{\mathbf{Q}}_{t-1} = \left[\tilde{\mathbf{H}}_{t-1} \mathbf{A}_t \hat{\mathbf{Q}}_t^{-1} \mathbf{A}_t^T \tilde{\mathbf{H}}_{t-1}^T + (\tilde{\mathbf{Q}}_{t-1} + \mathbf{U}_t)^{-1} \right]^{-1}, \qquad \tilde{\mathbf{H}}_{t-1} = (\tilde{\mathbf{Q}}_{t-1} + \mathbf{U}_t)^{-1} \mathbf{U}_t$$

starting with the last sample of the signal $t = N$, where $\hat{\mathbf{x}}_N = \tilde{\mathbf{x}}_N$, $\hat{\mathbf{Q}}_N = \tilde{\mathbf{Q}}_N$

Estimation of non-stationary regression coefficients as the universal problem of signal processing

$$y_t^0 = \mathbf{x}_t^T \mathbf{y}_t + \xi_t$$



Estimation of non-stationary regression coefficients in terms of the proposed optimization procedure

Signal to be processed	$(y_t^0, \mathbf{y}_t),\ y_t^0 \in \mathrm{R},\ \mathbf{y}_t \in \mathrm{R}^n,\ t=1,...,N$
Sought-for sequence of non-stationary regression coefficients	$\mathbf{x}_t \in \mathrm{R}^n$
Model of non-stationary linear regression	$y_t^0 = \mathbf{x}_t^T \mathbf{y}_t + \xi_t$

Local quadratic criterion for estimating the current vector of non-stationary regression coefficients (node functions):

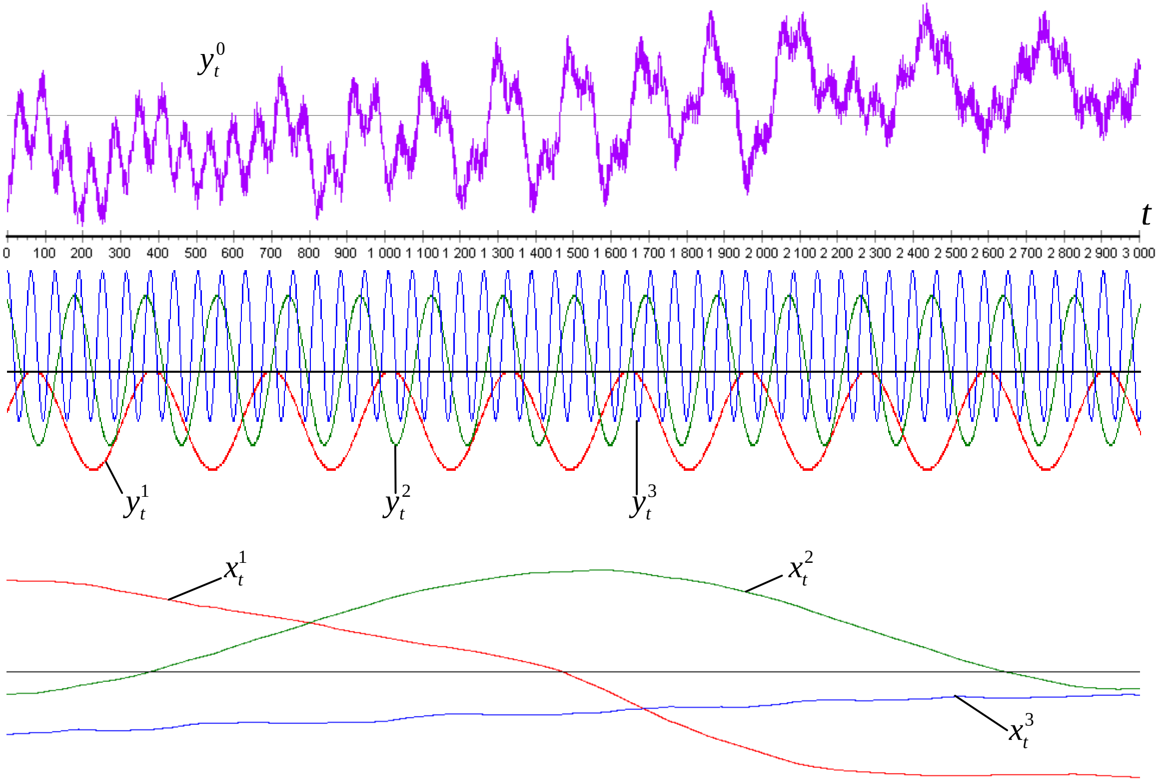
$$\psi_t(\mathbf{x}_t) = (y_t^0 - \mathbf{x}_t^T \mathbf{y}_t)^2 = (\mathbf{x}_t - \mathbf{x}_t^0)^T \mathbf{Q}_t^0 (\mathbf{x}_t - \mathbf{x}_t^0), \qquad \mathbf{x}_t^0 = \frac{y_t^0}{\mathbf{y}_t^T \mathbf{y}_t} \mathbf{y}_t, \qquad \mathbf{Q}_t^0 = \mathbf{y}_t \mathbf{y}_t^T .$$

Local quadratic penalty on unsmoothness of the sequence of non-stationary regression coefficient (edge functions):

$$\gamma_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = (\mathbf{x}_{t-1} - \mathbf{x}_t)^T \mathbf{U}_t (\mathbf{x}_{t-1} - \mathbf{x}_t),$$

$\mathbf{U}_t$ – an appropriate sequence of positive definite matrices $n \times n$, which preset the desired degree of smoothing at each pair of neighboring samples $(t-1,\ t)$

An example of estimating non-stationary regression coefficients



Smoothing of a signal with estimation of its differences

Model of the source signal:

$$y_t = \mathbf{x}_t^T \mathbf{y}_t + \xi_t$$

$\mathbf{x}_t = (x_t^1, ..., x_t^n)^T \in \mathrm{R}^n$ – vector composed from the smoothed signal itself and its first $n-1$ differences

$$x_t^1 = x_t$$

$$x_t^2 = \nabla^1 x_t = x_t^1 - x_{t-1}^1$$

$$\ldots$$

$$x_t^n = \nabla^{n-1} x_t = x_t^{n-1} - x_{t-1}^{n-1}$$

$\mathbf{y}_t = (1,0,...,0)^T \in \mathrm{R}^n$ – vector whose first component is unit and all the others are zeros

Model of the sought-for signal

$$x_{t-1}^1 = x_t^1 - x_t^2$$

$$x_{t-1}^2 = x_t^2 - x_t^3$$

$$\ldots$$

$$x_{t-1}^n = x_t^n$$

$$\mathbf{x}_{t-1} = \mathbf{A}\mathbf{x}_t, \quad \mathbf{A} = \begin{pmatrix} 1 & -1 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

Quadratic node functions:

$$\psi_t(\mathbf{x}_t) = (y_t - x_t^0)^2 = (\mathbf{x}_t - \mathbf{x}_t^0)^T \mathbf{Q}_t^0 (\mathbf{x}_t - \mathbf{x}_t^0)$$

$$\mathbf{Q}_t^0 = \mathbf{y}_t \mathbf{y}_t^T = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}, \qquad \mathbf{x}_t^0 = \frac{y_t}{\mathbf{y}_t^T \mathbf{y}_t} \mathbf{y}_t = \begin{pmatrix} y_t \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

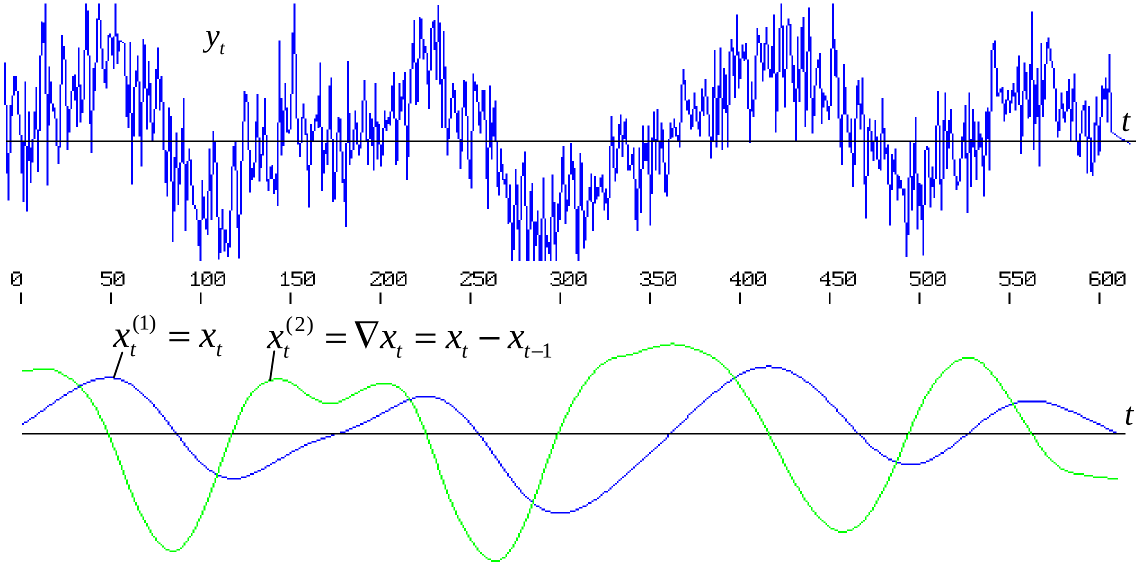
Quadratic edge function

$$\gamma_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = (\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t)^T \mathbf{U}_t (\mathbf{x}_{t-1} - \mathbf{A}\mathbf{x}_t),$$

$$\mathbf{U}_t = \begin{pmatrix} \beta u_t & 0 & \cdots & 0 \\ 0 & \beta u_t & \vdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_t \end{pmatrix}$$

where β is a large positive number $\beta \to \infty$.

Example of smoothing a signal and its first difference



Autoregression and time-frequency analysis

Source signal

$$y_t = \mathbf{a}_t^T \mathbf{y}_t + \xi_t$$

$\mathbf{y}_t = (y_{t-1} \cdots y_{t-n})^T$ – prehistory vector composed from n previous samples of the source signal

$\mathbf{a} = (a_1 \cdots a_n)^T \in \mathrm{R}^n$ – vector of autoregression coefficients

Sought-for vector signal

$$\mathbf{x}_t = (\mathbf{a}_t, D_t) \in \mathrm{R}^{n+1}$$

Quadratic node functions

$$\psi_t(\mathbf{a}_t, D_t) = \psi_t(\mathbf{x}_t) = (\mathbf{x}_t - \mathbf{x}_t^0)^T \mathbf{Q}_t^0 (\mathbf{x}_t - \mathbf{x}_t^0),$$

$$\mathbf{x}_t^0 = \begin{pmatrix} \mathbf{a}_t^0 \\ D_t^0 \end{pmatrix} = \begin{pmatrix} \dfrac{y_t}{\mathbf{y}_t^T \mathbf{y}_t} \mathbf{y}_t \\ y_t^2 \end{pmatrix} \in \mathrm{R}^{n+1}, \quad \mathbf{Q}_t^0 = \begin{pmatrix} \mathbf{y}_t \mathbf{y}_t^T & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} [(n+1)\times(n+1)]$$

Quadratic edge functions

$$\gamma(\mathbf{x}_{t-1}, \mathbf{x}_t) = (\mathbf{x}_{t-1} - \mathbf{x}_t)^T \mathbf{U}_t (\mathbf{x}_{t-1} - \mathbf{x}_t),$$

$$\mathbf{U}_t = \begin{pmatrix} u_t \mathbf{I} & \mathbf{0} \\ \mathbf{0}^T & \alpha u_t \end{pmatrix},$$

$\mathbf{I}$ is unit matrix $(n \times n)$, the coefficient $\alpha > 0$ is meant to coordinate the smoothing degrees for signal intensity D and autoregression parameters $\mathbf{a}_t$.

Spectral representation of autoregression parameters

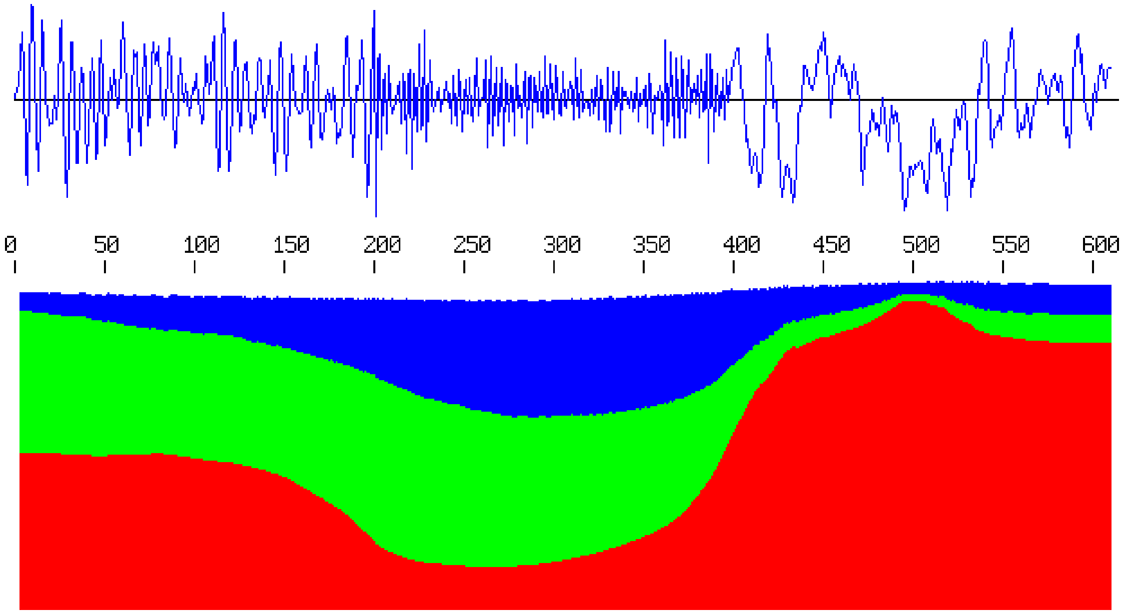
$$S(f)=\frac{(1+a_2)\left((1-a_2)^2-a_1^2\right)}{(1-a_2)}\frac{2D}{1+a_1^2+a_2^2-2a_1(1-a_2)\cos 2\pi f-2a_2\cos 4\pi f}$$

$$\hat{D}_t(0,1/6)=\int_0^{1/6}S(f;\hat{\mathbf{a}}_t,\hat{D}_t)df,$$

$$\hat{D}_t(1/6,1/3)=\int_{1/6}^{1/3}S(f;\hat{\mathbf{a}}_t,\hat{D}_t)df,$$

$$\hat{D}_t(1/3,1/2)=\int_{1/3}^{1/2}S(f;\hat{\mathbf{a}}_t,\hat{D}_t)df.$$

Result of processing a simulated signal



low, medium, and high frequency bands